

# 中心实验室仪器使用心得专栏 III 期 飞行时间质谱仪

## 基本信息

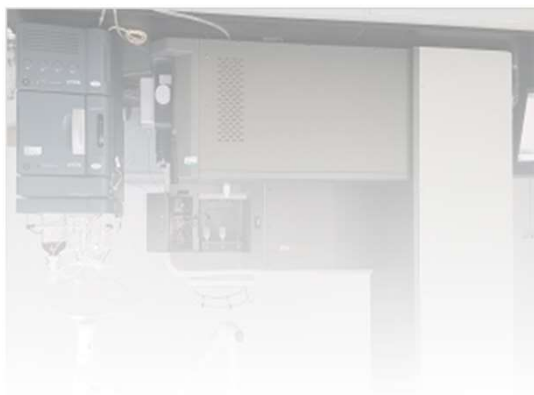


- 仪器型号：Waters Vion IMS Qtof
- 主要附件：与 Waters UPLC H-class 联用，配备 UNIFI 控制软件及代谢组学数据分析 QI 软件。

### ➤ 主要参数：

1. 四极杆质量范围： $m/z$  20-8,000; TOF 质量范围： $m/z$  20-100,000。
2. 分辨率： $\geq 40,000$  FWHM
3. 质量精确度，外标法 MS 及 MS/MS 模式达到  $< 1$  ppm。
4. 灵敏度（全扫描模式）：1 pg 利血平，柱上进样，MS 模式下，30 张图谱/秒的采样速率下， $S/N \geq 15000:1$ 。
5. 谱图内动态范围：5 个数量级。
6. 数据处理系统：仪器控制采集软件及代谢组学软件。

## 主要应用



## 成果展示

-----投稿人：刘敏

基本信息

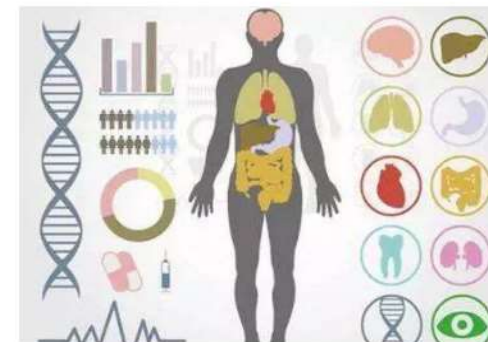
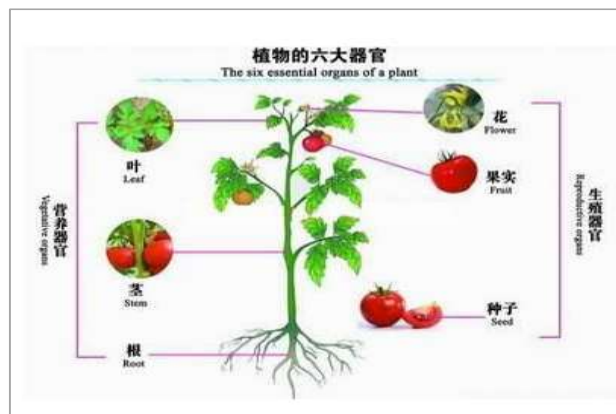
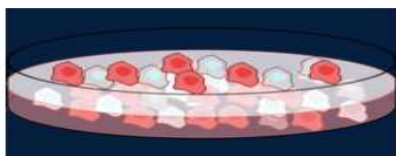
食品安全

天然产物及功能因子鉴定

未知化合物  
筛查

代谢组学研究

主要应用



成果展示

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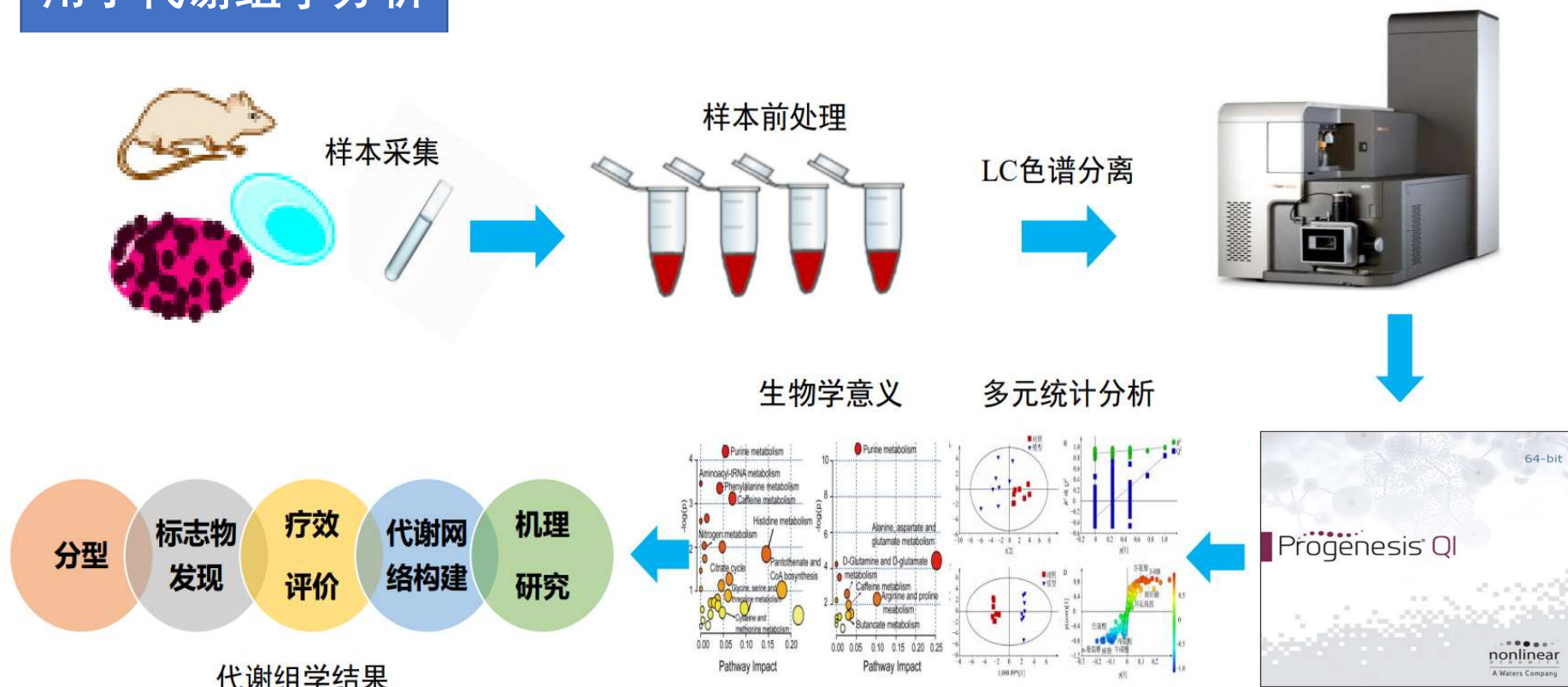
# 中心实验室仪器使用心得专栏 III 期 飞行时间质谱仪

基本信息

用于代谢组学分析

代谢组学

成果展示



QI预处理数据

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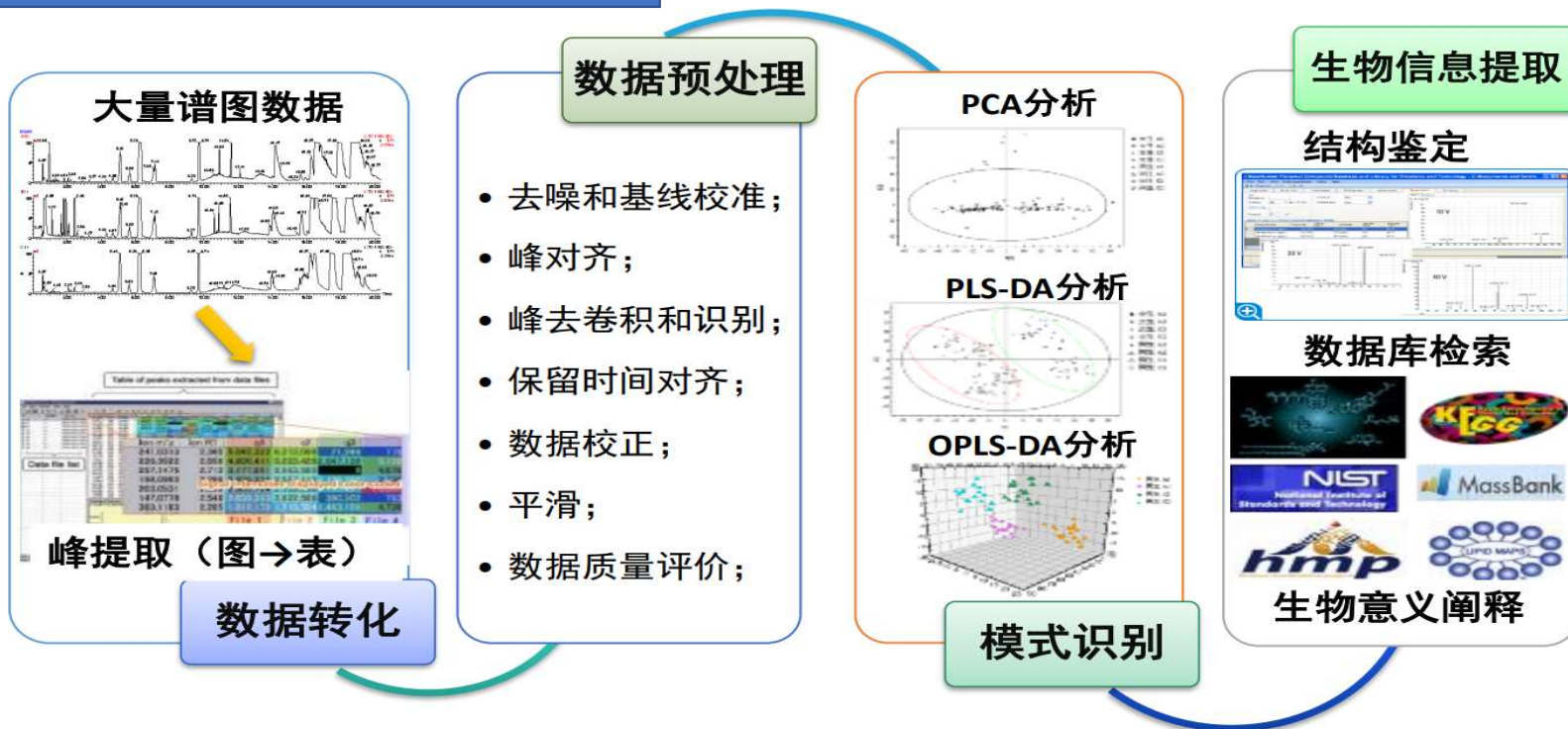
# 中心实验室仪器使用成果展 飞行时间质谱仪

基本信息

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## 质谱——数据处理全步骤



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# 中心实验室仪器使用成果展 飞行时间质谱仪

基本信息

Q1 处理过程



代谢组学

导入数据  
多种格式

- 1.Waters(.raw)
- 2.Thermo(.raw)
- 3.ThermoFT-ICR(.raw)
- 4.mzXML file

数据对齐  
三种模式

- 1.所有数据源中选择数据对齐参照(推荐使用)
- 2.在指定数据源中选择数据对齐参照
- 3.在数据源作为对齐参照

试验分组

根据实验分组进行分组即可

峰提取

根据实际情况选择参数

峰去卷积和识别

识别并量化信号,并使之与样品中的代谢物一一对应。

代谢物鉴定

通过数据库鉴定样品中的代谢物。

常用数据库:  
HMDB数据库  
LIPID MAPS数据库

成果展示

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# 中心实验室仪器使用成果展 飞行时间质谱仪

基本信息

代谢通路分析

QI中鉴定得到得差异代谢物导入KEGG数据库中中进行代谢通路分析

代谢组学

成果展示

Choose one of the following options to proceed

— A one-column compound list

### Data Input

Please enter a one-column compound list:

Input Type: — Please specify

Use our excel

- Compound Name
- HMDB ID
- KEGG ID

— A concentration table

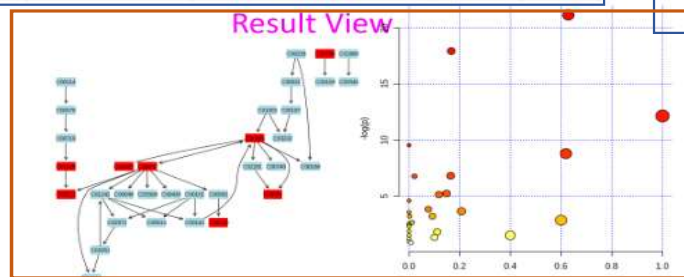
### Compound Name matching

Query	Hit	HMDB	PubChem	KEGG	Details
Acetoacetic acid	Acetabacetic acid	HMDB0000060	98	C00154	
Beta-Alanine	Beta-Alanine	HMDB0000058	239	C00099	
Creatine	Creatine	HMDB0000064	586	C00300	
Dimethylglycine	Dimethylglycine	HMDB0000092	673	C01026	
Fumaric acid	Fumaric acid	HMDB0001134	444972	C00122	
Olycine	Olycine	HMDB0000123	750	C00037	
Homocysteine	Homocysteine	HMDB0000742	778	C05330	

### pathway analysis

Mammals

- Select a pathway library
  - Homo sapiens (KEGG)
  - Homo sapiens (SMPDB)
  - Mus musculus (KEGG)
  - Mus musculus (SMPDB)
  - Rattus norvegicus (rat) (KEGG)
  - Bos taurus (cow) (KEGG)
- pathway analysis algorithms



Pathway Name	Match Status	p	-log(p)	Holm p	FDR	Impact	Details
<a href="#">Glycine and Serine Metabolism</a>	7/50	1.0070E-5	11.505	9.9786E-4	9.9786E-4	0.11953	<a href="#">KEGG SMP</a>
<a href="#">Methionine Metabolism</a>	5/29	2.8744E-5	10.423	0.0029149	0.0013998	0.11293	<a href="#">KEGG SMP</a>
<a href="#">Phenylalanine and Tyrosine Metabolism</a>	5/25	4.2417E-5	10.068	0.0041145	0.0013998	0.22124	<a href="#">KEGG SMP</a>
<a href="#">Homocysteine Degradation</a>	3/7	1.5995E-4	8.7406	0.015355	0.0039588	0.0	<a href="#">SMP</a>
<a href="#">Ammonia Recycling</a>	3/25	0.0085847	4.7578	0.81554	0.16998	0.0	<a href="#">KEGG SMP</a>
<a href="#">Alanine Metabolism</a>	2/14	0.024105	3.7253	1.0	0.34091	1.0	<a href="#">KEGG SMP</a>
<a href="#">Betaine Metabolism</a>	2/18	0.038852	3.248	1.0	0.42538	0.13201	<a href="#">SMP</a>

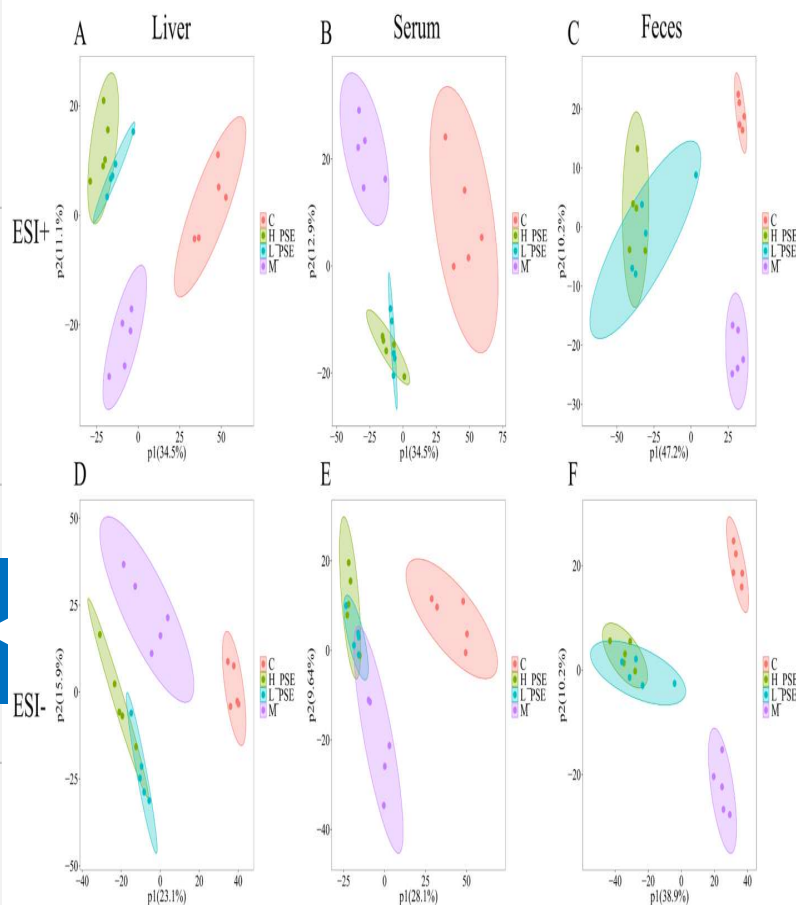
-----投稿人：刘敏

# 代表性成果 I：ApoE<sup>-/-</sup> 小鼠肝脏、血清和粪便代谢组分析

基本信息

主要应用

成果展示



**Title:** Peanut skin extract ameliorates high-fat diet-induced atherosclerosis by regulating lipid metabolism, inflammation reaction and gut microbiota in ApoE<sup>-/-</sup> mice

**Journal:** Food Research International, If: 7.425

**Methods:** metabolomics analysis, the raw data obtained from UPLC-Q/TOF-MS were typically pre-processed to provide structured data in an appropriate format for data analysis. First, the raw data were processed by the metabolomics processing software Progenesis **QI software** for baseline filtering, peak identification, integration, retention time correction, peak alignment and normalization.

**Result:** Different treatment groups could be evidently separated by PLS-DA based on the metabolites in the liver, serum and fecal samples in both ESI+ and ESI- modes, indicating that there were significant differences in metabolic phenotypes among the experimental groups.

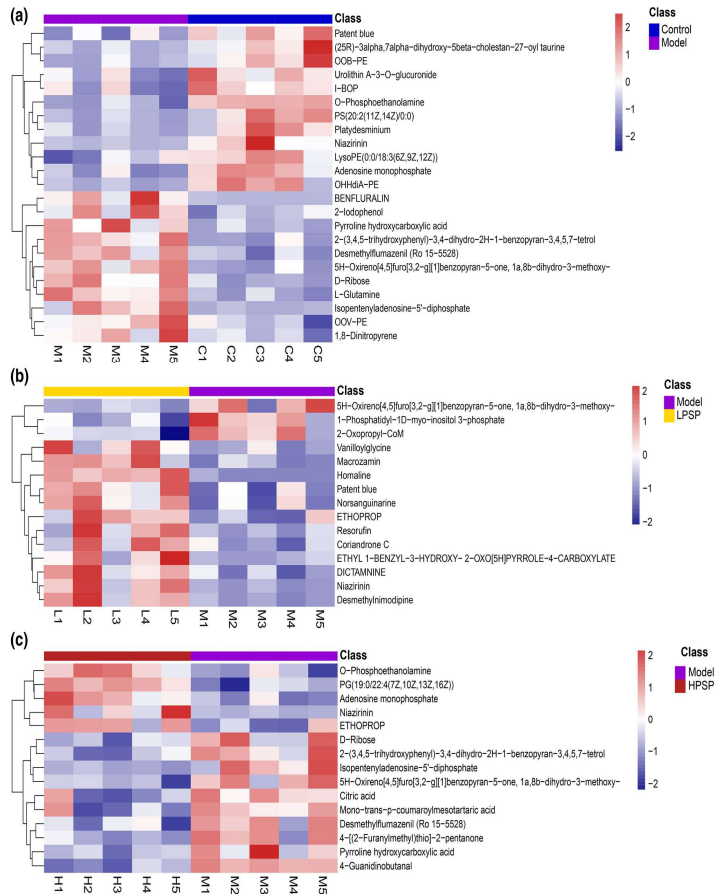
作者介绍：第一作者为许铭娟，通讯作者为刘睿教授

# 代表性成果II: colitis 小鼠结肠组织代谢组分析

基本信息

主要应用

成果展示



**Title:** The underlying mechanism of A-type procyanidins from peanut skin on DSS-induced ulcerative colitis mice by regulating gut microbiota and metabolism

**Journal:** Journal of Food Biochemistry, If: 3.654

**Methods:** All samples (50 mg) were homogenized together with 20  $\mu$ L internal standard (2-chloro-1-phenylalanine in methanol, 0.3 mg/mL) and 400 $\mu$ L extraction solvent with methanol /water (4/1, v/v), then vortexed for 1 min. Samples were sonicated for 10 min on ice and then placed at -20  $^{\circ}$ C for 30 min, and then centrifugation at 13,000 rpm for 10 min at 4  $^{\circ}$ C. The supernatants were collected for UHPLC-Q-TOF/MS analysis. The metabolome data were processed using Progenesis Q1.

**Result:** A total of 42 different metabolites were identified, and these metabolites indicated that PSP alleviated UC mainly correlated with taste transduction, mTOR signaling pathway, PI3K-Akt signaling pathway, and FoxO signaling pathway

**作者介绍:** 第一作者为黄碧君, 通讯作者为刘睿教授